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Using molecular simulation to explore unsually low moisture uptake in amine-cured epoxy carbon fibre reinforced nanocomposites

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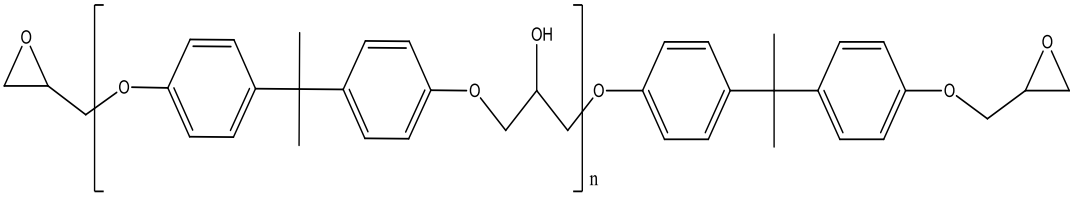
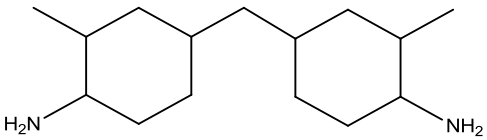
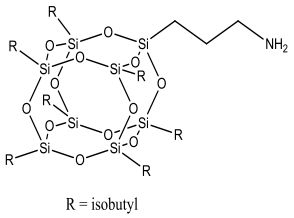


DGEBA



Dimethyl-methylene *bis*(cyclohexylamine)



Aminopropylisobutyl POSS)

Scheme S1. Structures of the reagents used in this work.

Table S1 Composition of the blends studied in this work

Sample	**Blend component g (mol.)**		
	DGEBA	**Dimethyl-methylene *bis*(cyclohexylamine)**	**POSS**
DGEBA	10.0 (5.6×10^{-2})	3.4 (1.4×10^{-2})	-
DGEBA-POSS$_{0.5\%}$			0.067 (7.7×10^{-5})
DGEBA-POSS$_{1\%}$			0.134 (1.5×10^{-4})
DGEBA-POSS$_{2\%}$			0.268 (3.1×10^{-4})
DGEBA-POSS$_{4\%}$			0.536 (6.1×10^{-4})

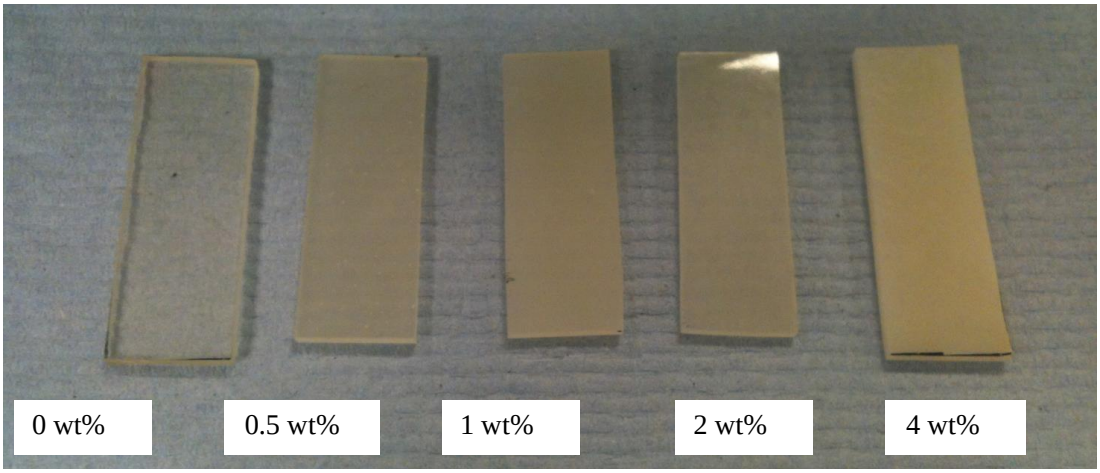


Fig. S1 Images of POSS in the DGEBA-amine system

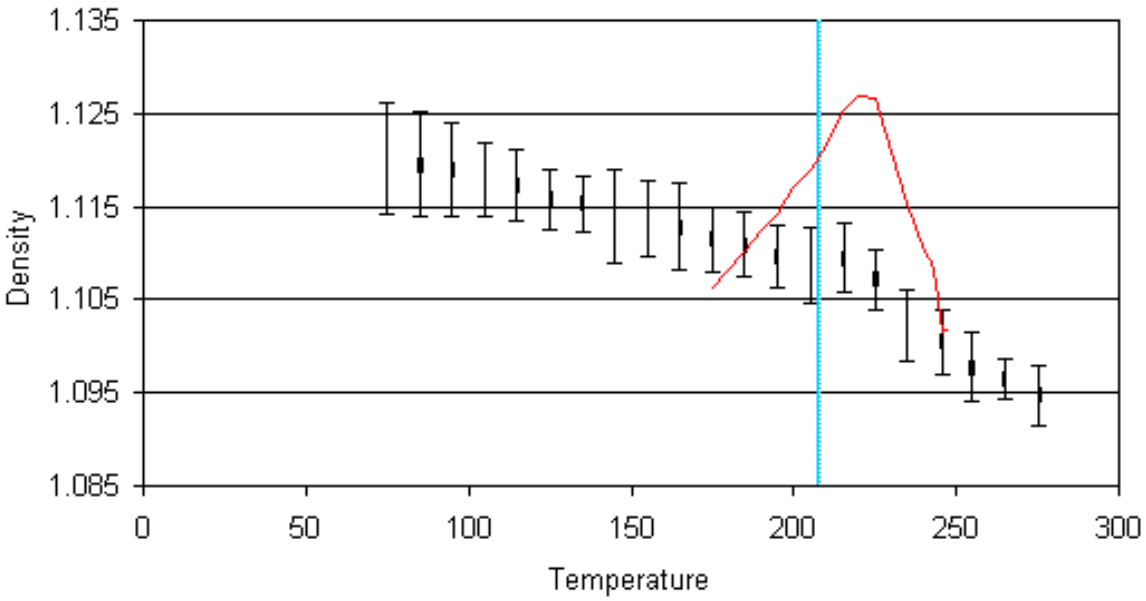
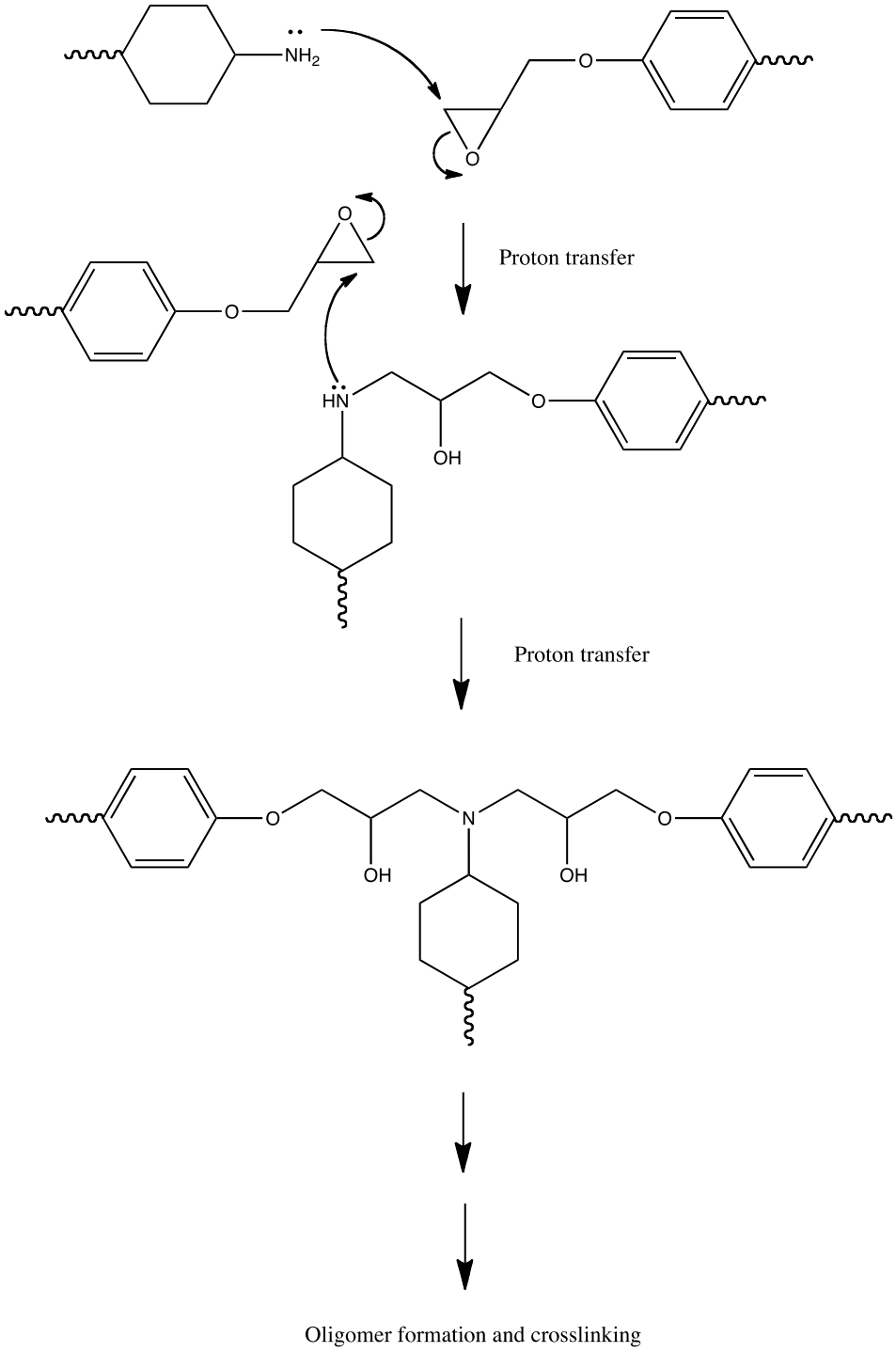


Fig. S2 Example data set showing MD raw data (black) and quality of fit (red).



Scheme S2. Initial stages of the amine-epoxy reaction, showing one half of the reagents (ref: I. Hamerton. Recent Developments in Epoxy Resins, Vol. 8 in Rapra Review Reports, R. Dolbey, Ed. RAPRA: Shropshire (1996).)

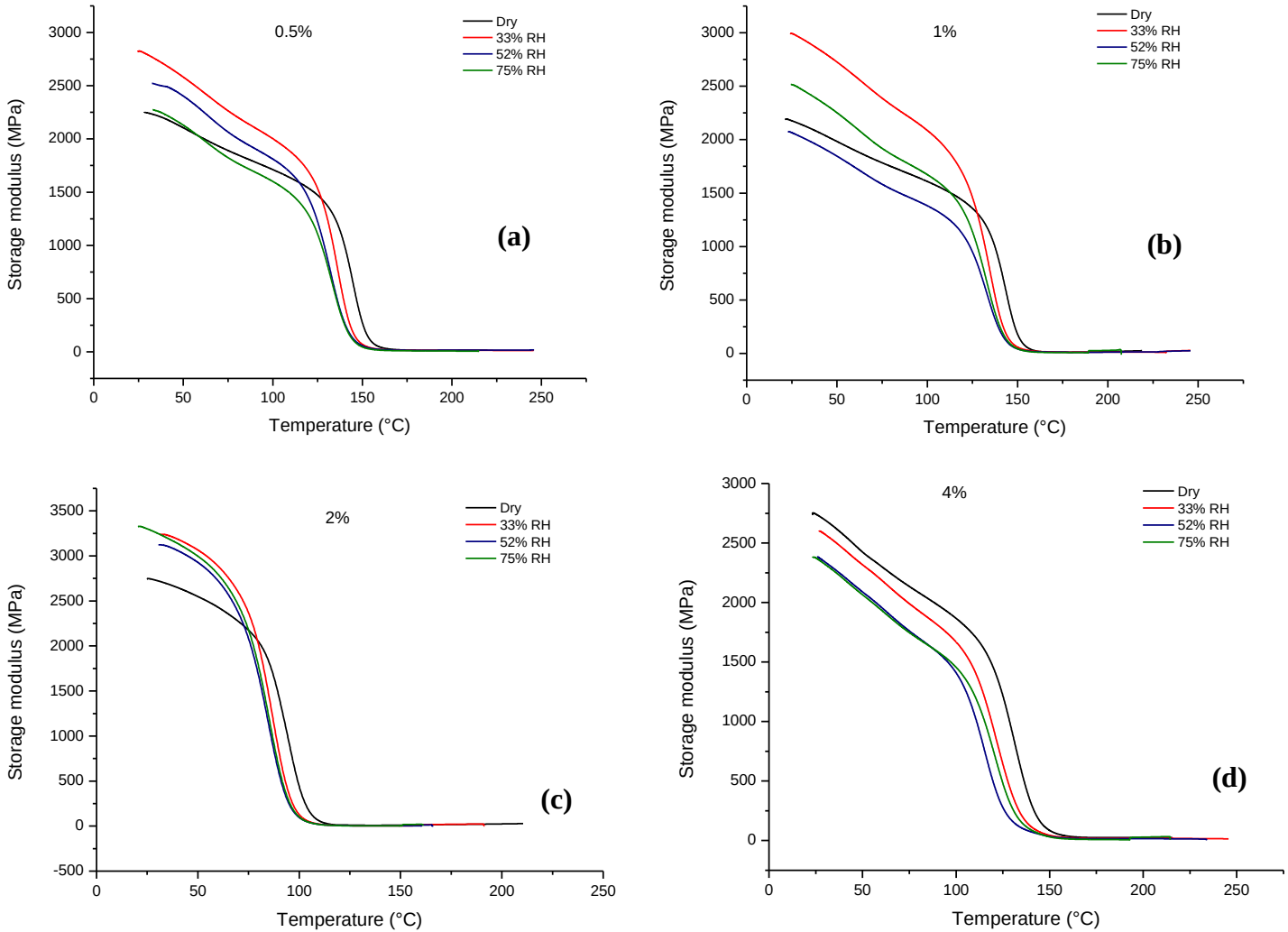
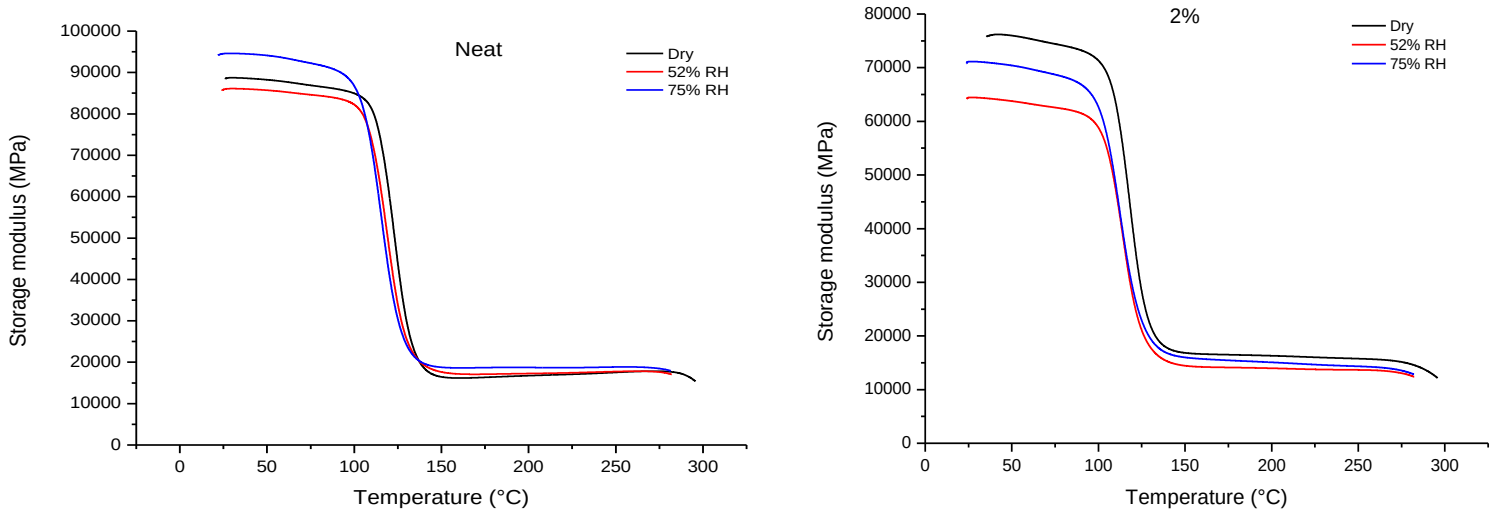

0.5%
Dry
33% RH
52% RH
75% RH
Storage modulus (MPa)
Temperature (°C)
(a)
1%
(b)
2%
(c)
4%
(d)

Fig. S3 Changes in storage modulus as a function of temperature at varying humidities of **(a)** 0.5% **(b)** 1% **(c)** 2% and **(d)** 4% DGEBA-POSS samples.



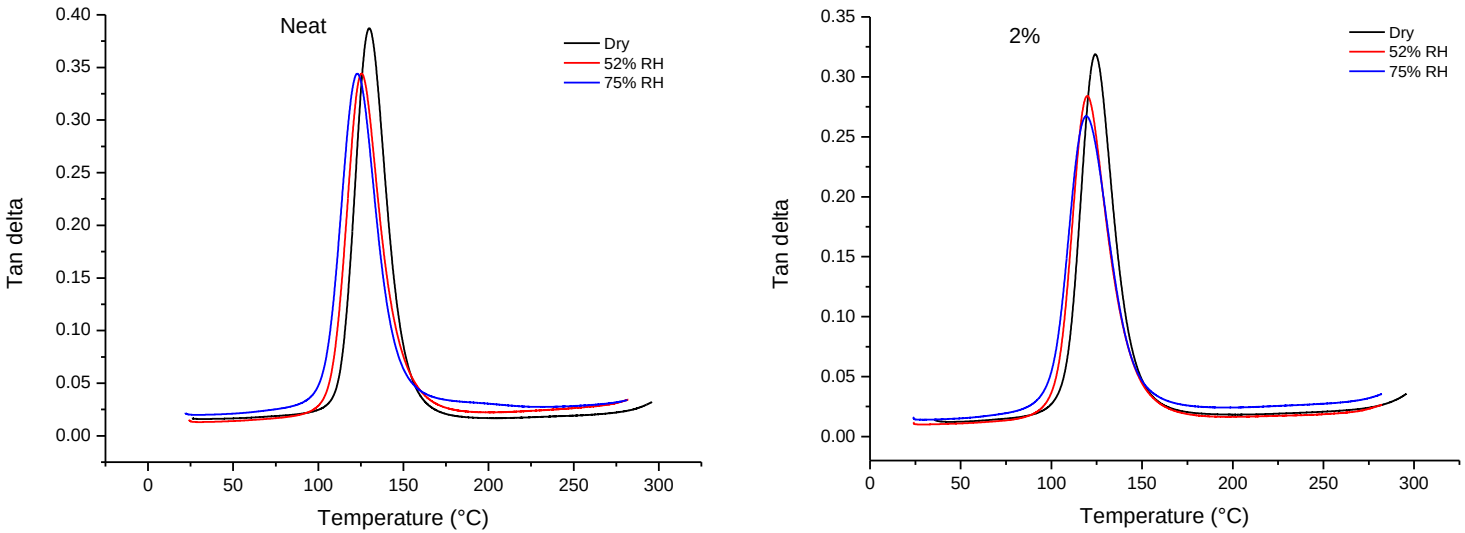


Fig. S4. Changes in storage modulus (top) and tan delta (bottom) of C(DGEBA) and C(DGEBA-POSS$_{2\%}$) following moisture conditioning.